AD-A094 042 XEROX PALO ALTO RESEARCH CENTER CA F/G 20/12
ANNUAL CONFERENCE ON THE PHYSICS OF COMPOUND SEMICONDUCTOR INTE--ETC(U)
1979 R S BAUER N00014-78-C-0728

UNCLASSIFIED NL

1 OF
AD
A094 042

END
DATE
FILMED
2-81
DTIC

LEVEL II

12

Final Report to the Office of Naval Research and the Army Research Office

AD A094042

Contract No. N00014-78-C-0728

SIXTH ANNUAL CONFERENCE ON THE PHYSICS OF COMPOUND SEMICONDUCTOR INTERFACES

Submitted by

R. S. Bauer

Xerox Palo Alto Research Center
3333 Coyote Hill Rd.
Palo Alto, CA 94304

On behalf of the Organizing and Program Committee
(see proposal for list of names)

1979

Chairman, Organizing and Program Committee

Robert S. Bauer
(415) 494-4118 (4000)

I. SUMMARY

A. *Title*: [redacted] ANNUAL CONFERENCE ON THE PHYSICS OF COMPOUND SEMICONDUCTOR INTERFACES

B. *Time and Place*: January 30-February 2, 1979, Asilomar Conference Grounds, 800 Asilomar Blvd., Pacific Grove, California 93950

C. *Costs*: Contract Budget: $17,500
Actual Expenses: $17,459

D. *Organizing and Program Committee*:

R. S. Bauer, Chairman, Xerox
C. R. Crowell, USC
R. Dingle, Bell
D. K. Ferry, Colo. State
J. L. Freeouf, IBM
J. D. Joannopoulos, MIT
B. D. McCombe, NRL
T. C. McGill, Cal-Tech
C. J. Nuese, RCA
W. E. Spicer, Stanford
C. W. Wilmsen, Colo. State

Ex-Officio:

L. R. Cooper, ONR
M. A. Littlejohn ARO
H. R. Wittmann, ARO
P. Mark, Proc. Ed., Princton

E. *Abstract*: Funds were used to support the Sixth Annual Conference on the Physics of Compound Semiconductor Interfaces which was held January 30 - February 2, 1979 at a self-contained Conference Center located at the Asilomar State Beach on the Monterey California Peninsula. This year particular emphasis was given to the fundamental inter-relationships between electronic, crystallographic, chemical, and metallurgical properties and growth and defect structures at semiconductor surfaces and interfaces. The meeting was attended by 240 scientists from 27 states and 11 foreign countries with 60% representing industrial organizations.

II. DISCUSSION

A. *Background*:

The surface and interface properties of intermetallic III-V and II-VI compound semiconductors are becoming increasingly important in practical technology in such wide-ranging fields as planar electronic device technology, light-emitting and light-detecting devices, energy conversion devices, large-volume semiconductor power devices and chemical catalysis. These involve interfaces of the semiconductor with insulators, metals, vacuum, electrolytes, and other semiconductors. Many, if not most, of the surface and interface properties of these materials are not fundamentally understood either theoretically or experimentally. The basic questions involved include atomic composition, crystallographic order, electronic structure, chemical activity, electronic transport, atomic diffusion, interfacial metallurgy, epitaxial growth, gas-solid induced conductivity modulation, electrical contact formation, and others. Clearly, these material properties find very wide exploitation in practical technology even if they are under sufficient empirical control in certain isolated cases to make the fabrication of certain devices a practical reality.

The purpose of this conference series is the study and discussion of fundamental properties of semiconductor interfaces with the view of eventually bringing an understanding to device characteristics. This conference serves as a gathering point for active researchers in the general field of semiconductor surface and interface physics. It is organized to promote the exchange of ideas and to develop strenthened lines of communication. While most of the presentations are specifically directed towards compound semiconductor interfaces, fundamental work on elemental semiconductor interfaces is included where it provides valuable insight for general interface properties.

B. *Objectives*:

Support was used to help organize the conference by contributing to certain costs such as secretarial help, office expenses (telephone, mail, duplicating, printing), travel assistance for invited speakers and students, travel assistance for meetings of the Organizing and Planning Committee, and underwriting publication costs of the conference proceedings. The remaining financial support was derived from attendance registration fees.

C. *Organization*:

The organization of the conference was built on the experience of the previous conferences. The business of the meeting lasted three days with flexible format and only one parallel session. The novel format which allowed 96 papers is discussed in the next section. The conference was held at the Asilomar Conference Grounds, 800 Asilomar Blvd., Pacific Grove, CA 93950 on January 30, 31, and February 1, 1979, with February 2 designated as the departure date. Adequate space and flexible facilities were available for completely serving all of the conferences needs. Attendance at the conference was required unless special circumstances warranted an exception. Fees for housing and meals included the costs for four nights' lodging, all meals from Monday dinner through Friday breakfast, evening hospitality, and one excursion. In order to avoid penalty charges for unused facilities, a $10 late fee was required of those making arrangements after December 29. A $10 fee was added to bills that are not paid before the start of the conference.

The Organizing and Planning Committee consisting of 14 scientists held two formal meetings and four informal gatherings in preparation for the conference. The first was on April 18, 1978, in Chicago to critically analyze the Fifth Conference and choose areas for particular emphasis at the forthcoming conference. Two weeks after

the October 27, 1978, abstract submission deadline, the committee met again, in Dallas, Texas, to evaluate the papers, choose invited speakers, and fix the format for the various topics within the semiconductor interface field. It was essential that the entire committee attend both meetings and that the necessary financial subsidy of these expenses was fully covered.

The *Proceedings* are published in the **Journal of Vacuum Science and Technology** (JVST) as the 1979 September/October issue (#5) of Volume 16, pages 1101 through 1533. The manuscript contributions have a length limit of 3000 words for contributed papers and 5000 words for invited papers. All contributions underwent anonymous review in conformity with standard JVST policy.

D. *Conference Format*:

When a 3-day meeting only contains a couple of dozen papers and perhaps twice that number of participants, it is not difficult to allow adequate discussion time and stimulate frank interchanges. To obtain a broader representation of diverse experiences and viewpoints, one quickly finds that a larger group is involved. Throughout the past year, the Organizing Committee for this conference wrestled with various alternative formats for translating the spirit of a workshop into a 250-person conference. The goal was to limit the number of oral presentations which could be accommodated within the fixed time of the meeting so adequate discussion of the entire audience would be allowed. It was decided that discussion should last two-thirds as long as the time allotted to the talk in order to accommodate reasonable interchanges. This total was distributed among all the talks rather than specifically allocating a fixed time to each presentation. Consequently, the program did not show any times other than for the start of the session. This severely limits the number of papers that can be included in 3 days without parallel sessions. Yet simple poster sessions were deemed unacceptable since the advantages of open

discussion and frank questioning would not be incorporated into the mainstream of the meeting. To insure adequate discussion time within such a large program, a novel sesison format was conceived. The following summarizes the main features of mixing presentation types.

During the first half of each session, approximately a third of the papers (typically five) were given orally by the authors; the remainder were summarized and a perspective of the work given by *Rapporteurs*; the choice was made by the committee strictly on the basis of topicality and not quality. The second part of each session was devoted to individualized and group discussion. This began with the break for refreshments. All authors, including those who had just made oral presentations, had assigned places around the perimeter of the meeting room. Those authors who did not make an oral presentation had a poster detailing their work. These displays were located in the conference hall during the entire day of presentation; they were also available for perusal and discussion throughout the meeting in other rooms. It is important to appreciate that successful communication by means of a poster depends on both the preparation of well-conceived, interesting, and informative displays and the principles followed by the browsing attendee. The session was reconvened by the *Moderator* for the last half-hour or so for a general discussion of all papers in the session. The *Rapporteurs* would often lead the discussion by raising questions of general interest.

The conference committee met six times to devise this format which would promote the exchange of ideas and develop strengthened lines of communication among active researchers in the general field of semiconductor surfaces and interfaces. In this spirit, papers were categorized topically and the final program organized to focus on a limited number of emerging issues where consensus did not presently exist and in-depth examination might be most profitable. Nearly a quarter

of the submissions were not accepted on the basis that their subject matter would not receive emphasis at this time. Still, PCSI-6 contained 40% more papers than last year and the organized discussion time was increased to occupy 40% of the conference.

The limitation of the mixed format to accommodate only five oral presentations per session, having an average length of 12 minutes each, was overwhelmingly perceived as an optimum situation. The procedure of gathering together as a large group for collective discussion following the poster period in each session had variable results but overall appeared to be a valuable part of the meeting. In future conferences, more burden should be placed on contributors to provide the *Rapporteurs* with outlines and visual aids; this should reduce the very substantial burden on the *Rapporteurs* and lead to greater uniformity in the summaries and evaluations they deliver. The papers comprising the Proceedings were ordered by subject without regard for presentaiton method.

III. CONFERENCE SUMMARY

The papers and discussion during this year's meeting were characterized by a melding of viewponts on the various interfaces. Whether the interface was metal/semiconductor, oxide/semiconductor, or heterojunction, it is beginning to appear that properties of the compound semiconductor (whether chemical-interaction induced, defect induced, or intrinsically induced) control the characteristics of the interface. Much of the interplay between phenomena discussed for various interface types is the result of an increasing emphasis on a microscopic understanding of interface formation and the accompanying geometric and electronic structure changes. A prime example is the attempt at describing the mechanism responsible for Schottky barrier behavior. The experimental demonstration that substances such as GaAs have no intrinsic surface states within the forbidden bandgap has, in the past several years, caused many groups to attribute the Schottky barrier pinning observed for such materials to "chemical interactions" between the overlayer and the substrate. Such interactions were discussed from several viewpoints. The formation of compounds at the interface was reviewed by Ottaviani; Ho, et al., provided a detailed study of one such system. Skeath, et al., and Bachrach, et al., both observed intermixing between the substrate and the deposited overlayer; Skeath, et al., discussed Schottky barrier pinning in terms of the defects (e.g., vacancies) implied by such diffusion as well as an exchange reaction reported by both groups (Al on GaAs → Ga on AlAs on GaAs). Williams demonstrated how intermediate monolayers of adsorbed gases and disorder could alter the interface chemistry drastically, but have little influence on contact behavior. Experimental questions were raised on a number of reported properties such as the retification of both the (100) GaAs-AlGaAs n-n heterojunction [Garner, et al., and Chandra, et al.] and the Ga contact to p-type GaAs (100) [Bachrach, et al., and Skeath, et al.]. Intense discussions of experimental and theoretical methodology were also frequent as exemplified by examination of such careful work as Brillson's surface photovoltage measurements and Van Laar's tight-

binding calculations of angle-resolved photoemission. Interpretations were equally controversial with strong advocates for vacancy-controlled Schottky barrier pinning [Spicer, et al., and Williams], other reaction and diffusion-produced defects controlling metal contact behavior [Bachrach, et al.], submonolayer dipole layer formation followed by charge transfer [Brillson], and even intrinsic semiconductor surface states pulled into the bandgap by metal-induced surface structural rearrangements [Mele, et al., and Chadi, et al.]. The increased experimental activity now focused on these questions should provide greater consensus in the near future.

There has been a great deal of progress in understanding chemisorption and clean surface structure problems. Whereas the major discussion of PCSI 3 was the lack of intrinsic surface states within the bandgap of III-V semiconductors, there is now general agreement on this situation with Monch reporting the extrinsic origin of previously observed states. The core level photoemission evidence for the chemisorbed oxygen on GaAs (110) being molecular was revised at this meeting by Chye, et al., since chemical shifts of Ga (3d) electrons were now observed. In fact, a wide body of new work finds broad-based agreement that atomic oxygen is the monolayer chemisorbed species. The XPS studies of Brundle were the first photoemission results to consistently contain Ga (3d) core involvement, while Barton, et al., showed that theoretically, a single As adsorption site could be responsible for core shifts of both substrate constituents. The use of surface EXAFS to distinguish bonding geometries of adsorbates was reported by Stohr, et al.; their very short deduced bonding distance for atomic oxygen caused widespread interest and speculation on both analogous bulk oxides and the possibility for unique surface oxygen bonding when constraints imposed by the bulk are removed in the chemisorption problem. While oxygen chemisorption on GaAs (110) appears to be nearing understanding, Chen, et al., reopened the question on Si (111) by reporting that only atomic oxygen adsorption could explain photoemission, in disagreement with the

widely accepted peroxy-radical description of O_2 bonding at monolayer coverages.

This meeting included an extensive examination of the application and reliability of LEED by all the major groups working on semiconductor surfaces. Jona discussed the qualitative and quantitative testing methods used for determining agreement between theory and experiment. After many years of zeroing in on the structure of GaAs (110), there is surprisingly good agreement (to within 2° rotation) among all studies now. Chadi discussed an empirical tight-binding method for calculating total energies and how it can predict the most likely structures to be used as test models for LEED comparisons. Numerous interesting attempts at understanding the Si (111) 7x7 surface were reported with no clear indication yet as to whether a large quantity (~25%) of vacancies is necessary to describe this structure. A theoretically deduced buckled-dimer model was presented by Chadi for Si (100), with Jona discussing LEED and Himpsel and Eastman reporting the surface state dispersion for this surface. While there is no agreement yet on these Si structures, the lively discussions demonstrated the increasing array of techniques now being widely applied and the increasing interdependence of theory and experiment. This was perhaps most graphically evident in the assignment of numerous valence band photoemission features to surface states of GaAs (110) by Ludeke and Ley, which Colbert and Shevchik reported could all be explained by direct transitions in the <u>bulk</u> band structure.

The conference included a critical review of advances in theoretical methods and their applications. It was characterized by spirited discussion of the methods being used to study the electronic structure of surfaces and interfaces. Goddard and Messmer indicated how quantum chemists study chemisorption by considering suitably chosen molecular clusters, while Schluter and Pantelides showed how the solid state physicists make use of band structure methods to calculate localized surface and interface energy levels. Both groups stressed the desirability of developing new methods which would

combine the advantages of these mutually complementary approaches, but no concrete suggestions were offered. There was considerable discussion of the progress being made by self-consistent pseudopotential methods. But it was stressed by Haneman that these methods have been employed at different levels of approximation, leading to results having varying degrees of reliability. Herring raised the question whether existing or contemplated solid state methods actually yield accurate electronic charge distributions. It was hoped that the first-principles pseudopotentials now appearing in the solid state physics literature (this is already an old story to the quantum chemists) would open the door to meaningful total energy and optimum geometry calculations for surfaces. For a critical oveview of the theoretical state of the art, see the paper by Herman at the beginning of these Proceedings.

One of the most popular sessions considered interface properties in general, with several types of semiconductor interfaces discussed including internal grain boundaries. The use of spectroscopic ellipsometry for nondestructive characterization of interface layers was reported by Aspnes, et al. They examined plasma-oxidized GaAs and showed that a-As is present for fast oxidation but is converted to c-As upon annealing at 550°C in a nitrogen ambient. Further information on the oxidized GaAs surface was presented by G. P. Schwartz, et al., who used Raman scattering to evaluate anodically-grown oxides on GaAs. They observed that elemental arsenic is not an intrinsic bulk or interfacial oxidation product of room-temperature anodization, but that it does form near the oxide-semiconductor interface after an anneal at temperatures as low as 350°C. Woodall, et al., observed that anodic oxides formed in aqueous solutions exhibited lower recombination velocities than annealed anodic oxides. The formation of an elemental arsenic layer at the oxidized GaAs surface probably increases the density of interface states, as suggested by an enhanced surface recombination velocity. Casey, et al., reported the successful passivation of a GaAs p-n junction with an oxygen-doped AlGaAs layer deposited by molecular beam epitaxy. The close lattice-match reduced the

recombination velocity at the GaAs/AlGaAs interface offering an attractive alternative to the customary approach involving deposited native oxides on III-V materials. Several papers discussed the application of deep level transient spectroscopy (DLTS) as a new and powerful technique for semiconductor interface studies. Crowell and Alipanali addressed the analytical problem of extracting information from the transient response when the concentration of deep levels, whether interface states or bulk defects, is large relative to the shallow dopant concentration. They showed that the detection sensitivity in the current-transient mode increases as the response time decreases while the capacitance mode behaves conversely. Johnson, et al., observed from constant-capacitance DLTS that on both (100)- and (111)-oriented silicon the interface-state distribution is dominated by a broad peak centered approximately 0.3 eV above the silicon valence band maximum which, by hydrogenation studies, was assigned to Si dangling bonds. The broad use of DLTS is perhaps best exemplified by a late contribution of Spencer, et al., who used the rectifying properties of a grain boundary (bicrystal) in epitaxial GaAs to provide a depletion region for DLTS measurements.

Considerable effort in the past several years has gone into numerous attempts to form insulating layers on III-V compounds which possess, simultaneously, good interface electronic properties and good dielectric properties (high breakdown strength, low conductivity), and to understand the complex electronic properties exhibited by these structures. Results on GaAs by anodic oxidation and deposition of various insulators have been largely disappointing, and results reported at this conference were in keeping with this trend, although improved understanding is being achieved. However, it should be noted that some recent developments on plasma anodization of GaAs and oxidation of thin epitaxial films of AlAs and $Ga_{1-x}Al_xAs$ on GaAs, which have shown apparent improved characteristics, were not presented at the conference. The most promisng new developments were in the area of deposited films of SiO_2 at relatively low temperatures on InP and InSb. Both Lile, et al., and Stannard reported rather good results on SiO_2-

InP MIS structures (in the former case actual transistors, and in the latter case MIS capacitors). Inversion for p-InP was clearly demonstrated for the first time by surface channel conductivity measurements by Lile, et al.; both sets of authors eventually agreed that inversion as not achieved in n-InP due to a large density of "interface states" in the gap near the conduction band edge. However, results reported by Pande and Roberts on anodically oxidized n-InP MIS structures exhibited clear indications of inversion from low frequency C-V measurements. Excellent electrical properties for low temperature SiO_2 on n-InSb were described by Langan, et al. Spicer, et al., presented a microscopic model which attempted to correlate UHV measurements on InP and GaAs surfaces with the electronic properties of MIS structures on these materials. The model, based on interface defects caused by missing cations and anions, is controversial but nevertheless indicates a possible direction for understanding observed trends, and is the first serious attempt to obtain such a microscopic understanding.

The interface between different semiconductors presents perhaps the broadest range of possibilities for studying both novel quantum mechanical phenomena and fascinating materials science questions. There was continuing investigations of the Ge/GaAs heterojunction, the so-called ideal test case. Kraut, et al., reported detailed measurements of the interfacial dipole for different crystalline orientations. Pollman and Pantelides reported the extension to the Ge/GaAs system of their scattering-theoretic approach for calculating interface states, while Denley, et al., presented measurements of these states by angle-resolved photoemission. These papers reinforce the view that the interfacial properties are established with fractional coverage of Ge on GaAs, and that the interfacial region extends over only a few monolayers. Considerable interest is focused on the (100) GaAs-AlGaAs interface. Here a controversy exists between groups that are unable to achieve rectification at an n-n heterojunction and those who have observed rectification. Additionally, there is the question of: If an accumulated two-dimensional electron gas exists on the GaAs side of the interface, can rectification be expected?

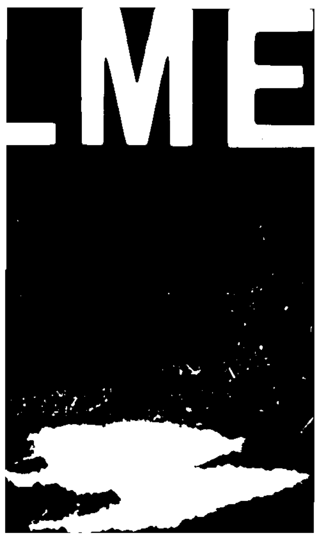
Currently, it appears that the presence of 2-D electron behavior does not bear strongly on the rectification question since it only demonstrates the presence of a "notch" in the band structure right at the interface. More important for rectification is the degree of doping on both sides of the junction, the sharpness of the interface and their affect on the overall band structure via band bending in the general vicinity of the junction. There was a general perception that the experimental particulars caused many of the discrepancies and that upon further study, there probably would be agreement that these n-n heterojunctions do rectify. Another key area of heterojunction investigation relates more to quantum mechanical and band structural effects in III-V superlattices and to the discussion of possible new superlattice systems with intriguing properties. The general trends, semimetal-semiconductor transitions, optical gaps, carrier confinement, etc., can be treated with rather simple models that are based upon the relative disposition of the VB, CB edges and upon E_g of the various superlattice components. There are systematic changes from the best studied GaAs-AlGaAs case through CdTe-HgTe to InAs-GaSb. These superlattice structures provide a sufficient perturbation of the bulk properties to promise new and intriguing phenomena and considerable experimental and theoretical activity.

Generally speaking, this conference continued the strong trend toward achieving a microscopic understanding of interface characteristics and behavior. Whether the advances were in our atomistic models of specific surfaces and interfaces or the thermochemistry and kinetics controlling interface formation, the experimental techniques and theory applied to compound semiconductors have become much more sophisticated in recent years. While only time will tell, the increased activity and cross-fertilization of many disciplines holds the promise for not only exciting science but also the engineering of new materials, device structures and phenomena.

IV. CONCLUSIONS

This series has become clearly recognized as one of the premier foci for the exchange of information in this field. Its success has led to a de-emphasis of semiconductor research at other major surface and interface science conferences (such as the annual meeting of the American Vacuum Society and the Physical Electronics Conference). The interest has grown to the point where novel organizational approaches have been taken to insure full discussion. The use of the remote, self-contained Asilomar conference site allowed experimentation in stimulating comprehensive analysis of emerging topics in this rapidly expanding field. This practice of providing all meals and entertainment as well as meeting facilities should be continued. The generous support of the ONR and ARO were vital in attracting the broad scientific participation and achieving the considerable success as judged by a survey of the conferees. The response of some 40% of the delegates to a questionnaire distributed at the close of the meeting suggests that the communication among participants was productive and profitable. Over 90% of the scientists found that PCSI 6 helped at least to some entent to generate new ideas for their research. In terms of both the time for discussion and the information exchanged, the discussion was rated good to excellent by nearly 90%; the previous 25% discussion allocation was generally inadequate. The scope, subject matter, and percentage of new results presented received a near-unanimous judgment that the scientific content was good to excellent. Interestingly, the 20% of time devoted to Si was viewed as beneficial by around 70% of the delegates attesting to the broad fundamental interest among those active in compound semiconductor research. While further optimization should certainly occur, the experiment with a mixture of presentation formats within a given session was a success. The funds provided by this contract allowed the conference committee to meet and formulate this novel meeting format, and they supported the travel expenses of key researchers, enabling

their attendence at PCSI 6.


LME